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FINAL REPORT

"LASER SPECTROSCOPIC STUDIES OF MOLECULAR CRYSTALS"

1 June 1975 - 30 November 1979

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1. PERSONNEL WHO PARTICIPATED IN THE RESEARCH

- Elliot R. Bernstein, Principal Investigator.
- Daniel L. Michalopoulos, Graduate Student Electronic Raman scattering and inorganic molecular vibronic coupling.
- 3. Gerald R. Meredith, Graduate Student ReF₆ magnetic properties, vibronic coupling, electronic Raman scattering and crystal vibrational levels.
- 4. John D. Webb, Graduate Student IrF₆ magnetic properties, vibronic coupling, electronic Raman scattering and crystal vibrational levels.
- 5. <u>John D. Webb</u>, Postdoctoral Fellow Nonlinear optical phenomena, multiphoton spectroscopy and photochemistry of C₃N₃H₃.
- Kerry M. Swift, Graduate Student Nonlinear optical phenomena multiphoton photochemistry and spectroscopy of OsO₄, C₃N₃H₃.
- Philip M. Kennedy, Graduate Student Nonlinear optical phenomena multiphoton photochemistry and spectroscopy of transition metal hexafluorides.
- 8. <u>K. M. Chen</u>, Graduate Student Spectroscopy of rare earth borohydrides, vibronic transitions in rare earth compounds.

II. TECHNICAL REPORTS GENERATED

- 7. "Spectroscopic Properties of Rare Earth Borohydrides: Er(BH₄)₃·3THF in Pure and Mixed Crystals," E. R. Bernstein and K. M. Chen.
- 8. "Interactions in Inorganic Molecular Crystals Electronic Spectra of ReF₆ Pure and Mixed Crystals," E. R. Bernstein and G. R. Meredith.
- 9. "Laser Optical Studies of Molecular Solids," E. R. Bernstein.
- 10. "On the Jahn Teller Effect in ReF₆," G. R. Meredith, J. D. Webb, and E. R. Bernstein.
- 11. "Raman Spectra of SiF $_4$ and GeF $_4$ Crystals," E. R. Bernstein and G. R. Meredith.
- 12. "Vibrational Spectra of Transition Metal Hexafluoride Crystals. I. Orthorhombic MoF_6 , WF_6 , and UF_6 Neat Crystals," E. R. Bernstein and G. R. Meredith.
- 13. "Vibrational Spectra of Transition Metal Hexafluoride Crystals. II.

 Two-Particle and Mixed Crystal Spectra as Techniques for Determination of Densities of States," E. R. Bernstein and G. R. Meredith.
- 14. "Vibrational Spectra of Transition Metal Hexafluoride Crystals. III. Exciton Band Structures of MoF_6 , WF_6 and UF_6 ," E. R. Bernstein and G. R. Meredith.

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II. (Continued)

- 15. "On the Jahn Teller Effect in IrF₆: The r_{8g} (t_{2g})³ State at 6800 Å," E. R. Bernstein and J. D. Webb.
- 16. "Charge-Transfer Interactions Between Transition Metal Hexafluorides and Xenon," J. D. Webb and E. R. Bernstein.
- 17. "Absorption and Electronic Raman Scattering Spectra of the $\Gamma 8g$ ($^2T_{1g}$) State of IrF_6 at 1.6 μ A Resolution of the Jahn Teller Problem," E. R. Bernstein and J. D. Webb.
- 18. "The Jahn Teller Effect in the Lowest Charge Transfer State of UF_6 ," E. R. Bernstein, G. R. Meredith and J. D. Webb.
- 19. "Raman Scattering of Neat and Mixed Crystals of IrF₆: The Jahn Teller Interaction in the Ground State," E. R. Bernstein and J. D. Webb.
- 20. "Quadratic Jahn Teller Coupling in Octahedral Systems," E. R. Bernstein and J. D. Webb.
- "A Ligand Field Theory Analysis of the Spectra of the t_{2g}³ Levels of IrF₆,"
 J. D. Webb and E. R. Bernstein.
- 22. "Two Photon Spectroscopy of Pyrazine and Triazine," J. D. Webb, K. M. Swift and E. R. Bernstein.

III. ACCOMPLISHMENTS

New results and new work our research has led to includes the following:

- a) Electronic Raman scattering in molecules.
- b) Magnetic phase transition in molecular solids (ReF6, IrF6).
- c) Elucidation of quadratic vibronic coupling (intra- and interstate) MF_6 , $C_3N_3H_3$.
- d) New insight into photochemical vs. fluorescence yields of excited states (C₃N₃H₃, C₄N₂H₄, OsO₄).
- e) Spectroscopy of cryogenic liquid solutions and energy transfer.
- f) Phase transition studies in molecular solids.
- g) Polariton behavior in molecular solids.
- h) Elucidation of vibrational mixing (normal mode breakdown) in degenerate electronic states (MF₆ systems).

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